

Unified Model of the Grüneisen Parameter, Melting Temperature, and Shear Modulus for a Compound

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A reliable model of the adiabatic (isentropic) shear modulus of a polycrystalline solid at temperatures up to the melting temperature, and up to megabar pressures is needed for many applications. It is generally assumed that the ratio of the plastic flow stress (shear stress necessary to induce plastic deformation at a given strain rate) to the shear modulus is approximately independent of pressure. In other words, the predominant pressure dependence of the plastic flow stress is contained in the shear modulus. An accurate, simple analytic (for fast evaluation) model of the shear modulus is therefore essential for numerical simulations of material deformation over extremes of pressure and temperature.

We have developed a new unified analytic model of the Grüneisen parameter, melting temperature, and shear modulus. It allows one to construct all three—the Grüneisen gamma, melting curve, and shear modulus—in terms of a common set of input parameters, thus providing independent tests for its validity, by comparing each of the three to the corresponding data.

Initially, the model was developed for simple elemental solids. Its reliability was proven by means of good-to-excellent agreement of the predicted melting curves and shear moduli to available experimental data and theoretical calculations on over a third of the elements in the periodic table.

More recently, the model has been generalized on compounds, that is, complex substances having two or more elemental constituents. The generalized model has been used to construct new SESAME melting curve and shear modulus tables for a number of compounds. In Fig. 1, a new SESAME melting curve for lithium fluoride (solid curve) is compared to the existing SESAME table (small points) and experimental data (large points). In Fig. 2, a new SESAME shear modulus for magnesium orthosilicate is compared to the experimental data on three solid phases of this compound (shown by points of different sizes).

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Acknowledgements

We would like to acknowledge NNSA's Advanced Simulation and Computing (ASC), Materials and Physics Program for financial support.

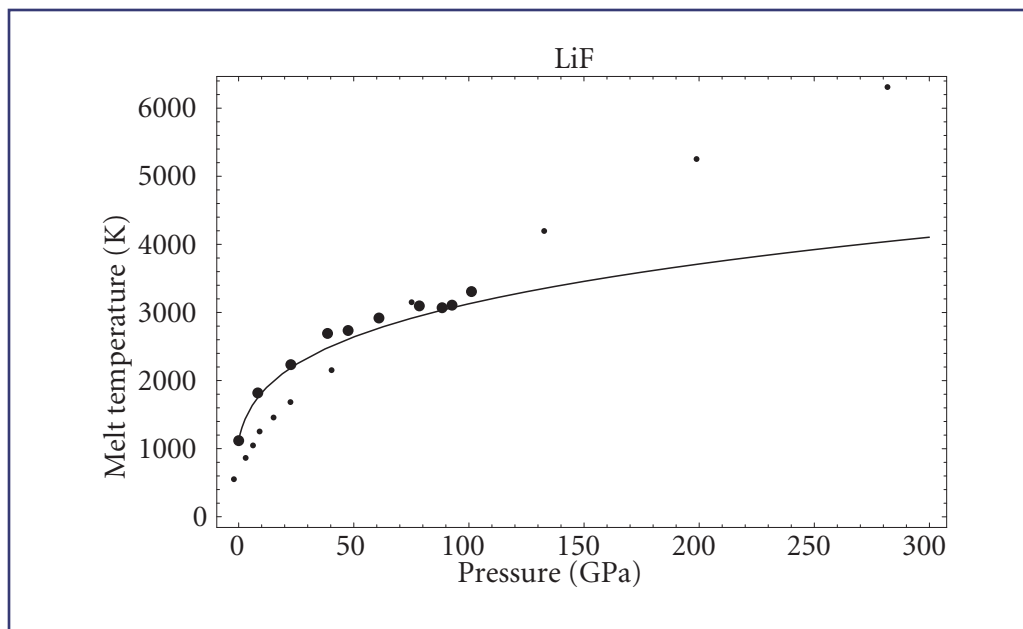


Figure 1—
A new SESAME melting curve for lithium fluoride (solid curve) is compared to the existing SESAME table (small points) and experimental data (large points).

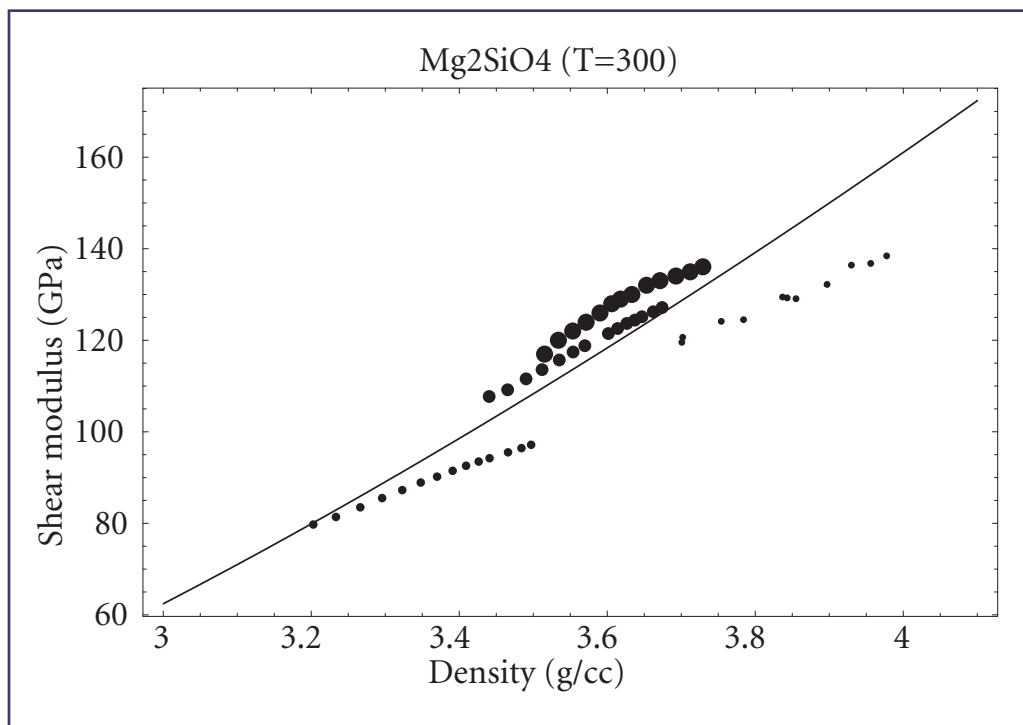


Figure 2—
A new SESAME shear modulus for magnesium orthosilicate is compared to the experimental data on three solid phases of this compound (shown by points of different sizes).